CONTENTS OF VOLUME 73

NUMBER 1—MAY 1991

EPR and ENDOR study on mixed crystals of an indolinone nitroxide radical and the isoelectronic ketone. I. X-ray structure of pure components and ENDOR of isolated radicals in mixed crystals
By A. L. Maniero, M. Brustolon, M. F. Ottaviani, C. Rizzoli, P. Sgarabotto, F. Ugozzoli, P. Carloni and L. Greci 1

EPR and ENDOR study on mixed crystals of an indolinone nitroxide radical and the isoelectronic ketone. II. EPR and ENDOR investigation on radical pairs in mixed crystals
By A. L. Maniero, M. Brustolon, M. F. Ottaviani, P. Sgarabotto and L. Greci 15

Relaxation phenomena in mixed isomeric alcohols by Mandelstam–Brillouin scattering
By D. Majolino, P. Migliardo, F. Aliotta, S. Magazú, C. Vasi, A. D'Aprano, D. I. Donato and V. Turco Liveri 27

Correlated studies of electric properties of ionic molecules: alkali and alkaline-earth hydrides, halides and chalcogenides
By P. W. Fowler and A. J. Sadlej 43

On the problem of detailed balance and model lineshapes in collision-induced rotovibrational bands: H_2–H_2 and H_2–He
By G. Birnbaum and A. Borysow 57

Collective motion and interparticle correlations in liquid water. A molecular dynamics simulation
By D. Bertolini, A. Tani and R. Vallauri 69

Neutron-diffraction investigation of the intramolecular structure of a water molecule in the liquid phase at high temperatures
By K. Ichikawa, Y. Kameda, T. Yamaguchi, H. Wakita and M. Misawa 79

An accurate integral equation for molecular fluids. I. Hard homonuclear diatomics
By S. Labík, A. Malijevský and W. R. Smith 87

An inelastic neutron scattering study of the dynamics of the van der Waals complex C_6H_6 : C_6F_6
By J. H. Williams 99

A quasielastic neutron scattering investigation of the van der Waals complex of benzene and hexafluorobenzene
By J. H. Williams 113

Excess properties of liquid mixtures from computer simulation: a coupling-parameter approach to the determination of their dependence on molecular asymmetry
By A. A. Chialvo 127

Molecular dynamics computer simulations of binary Lennard-Jones fluid mixtures: Thermodynamics of mixing and transport coefficients
By P. J. Gardner, D. M. Heyes and S. R. Preston 141

Towards an understanding of the static structure of suspensions of ionic rod-like macromolecules
By E. Canessa, B. D'Aguanno, B. Weyerich and R. Klein 175

Nematic, Smectic-A, and Smectic-C ordering in a system of parallel cylinders with quadrupolar interaction
By A. Poniewierski and T. J. Sluckin 199

Broadband excitation sequences for NQR spectroscopy
By A. Ramamoorthy and P. T. Narasimhan 207

On the 3d Rydberg states of the NO molecule
By A. Bernard, C. Effantin, J. D'Incan, C. Amiot and J. Vergès 221

Research Note

Secondary dissociation pathways of ethylsilylene radical on ground and excited state potential energy surfaces
By J. S. Francisco 235

NUMBER 2—JUNE 1991

Invited article: The spin-correlated radical pair as a reaction intermediate
By K. A. McLauchlan and U. E. Steiner 241

Potential energy functions for atomic solids. III. Fitting phonon frequencies and elastic constants of diamond structures
By A. R. Al-Derzi, R. L. Johnston, J. N. Murrell and J. A. Rodriguez-Ruiz 265

The structure of room temperature molten polyiodides
By L. A. Bengtsson, H. Stegemann, B. Holmberg and H. Füllbier 283

Third harmonic generation in molecular gases
By M. N. R. Ashfold and J. D. Prince 297

Rotationally inelastic rates and Raman Q-branch linewidths for $N_2 + N_2$
By P. J. Agg and D. C. Clary 317

***Ab initio* calculation of nuclear motion corrections to the geometries of water, methanol and silanol**
By J.-R. Hill, J. Sauer and R. Ahlrichs 335

Rotational relaxation rates for the $J = 0$–1 transition of N_2O by self-collisions and foreign gas collisions
By H.-W. Nicolaisen and H. Mäder 349

Percus-Yevick integral equation theory for athermal hard-sphere chains. II. Average intermolecular correlation functions
By Y. C. Chiew 359

An *Ab Initio* molecular orbital study of protonated water clusters, $H(H_2O)_n^+$ $n = 1$ to 5, at the SCF and MP2 levels
By E. P. F. Lee and J. M. Dyke 375

Neutron diffraction study of the partial pair correlation functions of liquid hydrogen sulphide
By C. Andreani, V. Merlo, M. A. Ricci and A. K. Soper 407

Equilibrium behaviour of quadrupolar Kihara molecule fluids
By T. Boublík 417

Quantum corrections to equilibrium properties of molecular fluids
By T. K. Dey and S. K. Sinha 427

Head–tail asymmetry and ferroelectricity in uniaxial liquid crystals. Model calculations
By F. Biscarini, C. Zannoni, C. Chiccoli and P. Pasini 439

Research Note

Parameterized dipole moment function for the water molecule
By M. A. Suhm and R. O. Watts 463

NUMBER 3—20 JUNE 1991

Computation of the transport coefficients of dense fluid neon, argon, krypton and xenon by molecular dynamics
By M. F. Pas and B. J. Zwolinski 471

Computation of the transport coefficients of binary mixtures of argon–krypton, krypton–xenon, and argon–xenon by molecular dynamics
By M. F. Pas and B. J. Zwolinski 483

An accurate integral equation for molecular fluids. Part II. Hard heteronuclear diatomics
By S. Labík, A. Malijevský and W. R. Smith 495

Monte Carlo simulation of the equilibrium partitioning of chain fluids between a bulk and a pore
By A. Yethiraj and C. K. Hall 503

Multiquantum resonances in low-field optically detected ESR of radical-ion pairs
By V. A. Morozov, O. N. Antzutkin, A. V. Koptyug and A. B. Doktorov 517

On the structure factor of liquid-like ordered binary mixtures of colloidal suspensions
By W. Härtl, C. Segschneider, H. Versmold and P. Linse 541

NMR in molecular crystals. An example: fluoroadamantane $C_{10}H_{15}F$
By R. Decressain, J. P. Amoureux, L. Carpentier and J. B. Nagy 553

The configuration and the dynamics of the $-CD_3$ groups in methyl deuterated dimethylmalonic acid. A single crystal deuteron NMR study
By S. Idziak, U. Haeberlen and H. Zimmermann 571

The liquid-phase structure of the tetrabromomethane–toluene complex. A differential anomalous X-ray scattering study
By T. Mager, H. Bertagnolli, D. Degenhardt and R. Frahm 587

Xenon adsorption in NaA zeolite cavities
By A. V. McCormick and B. F. Chmelka 603

Experimental orbital momentum distributions and bonding interactions. Part II. The organometallic complex $(\eta^4\text{-}1,3\text{-}C_4H_6)\text{–}Fe(CO)_3$
By K. McMillan, M. A. Coplan, J. A. Tossell and J. H. Moore 619

Transition probabilities in collisions between an atom and an anharmonic oscillator
By J. Récamier and J. Ortega 635

Potential energies and IR spectra for homopolar diatomic adsorbates over ion-exchanged ZSM-5 zeolites
By T. Yamazaki, I. Watanuki, S. Ozawa and Y. Ogino 649

A molecular dynamics simulation of HCl. A study of the vibrational dephasing mechanism
By A. Laaksonen and P.-O. Westlund 663

Linear relations between vibrational energy levels of CO_2 and fourth order spectroscopic constants
By G. Amat 685

Potential parameters of methyl and methylene obtained from second virial coefficients of n-alkanes
By A. López Rodríguez, C. Vega, J. J. Freire and S. Lago 691

Analytical solution of Wertheim's OZ equation for the Smith–Nezbeda model of associated liquids
By Y. V. Kalyuzhnyi and I. Nezbeda 703

NUMBER 4—JULY 1991

Atomic pair correlations in Lennard-Jones fluids: Analysis in terms of structural diffusion models
By L. Gutman and S. Baer 715

Stretching density of states of the deuterium sites in polycrystalline D_2O
By C. Andreani, J. Mayers, P. Postorino and M. A. Ricci 737

On the self-consistent equation for the microscopic local electric field in dielectric systems
By V. Mazzacurati and G. Ruocco 745

Hard dumbell fluid g_1 and g_2 from Monte Carlo
By D. J. Adams 757

Irreducible rational approximants for the hard-sphere fluid
By D. A. de Lonngi and P. A. Lonngi Villanueva 763

New analytical and numerical results on virial coefficients for 2-D hard convex bodies
By G. Tarjus, P. Viot, S. M. Ricci and J. Talbot 773

Free energy functionals and the structure of the uniform hard-sphere fluid
By G. P. Brenan and R. Evans 789

Two mechanisms of sensitization of photoconductivity in carbazole-containing polymeric semiconductors by Rhodamine 6G
By N. G. KUVSHINSKIJ, V. M. KOMKO and S. E. KOSTJUK 805

Hyperfine structure investigations of the excited AO^+ state of TlI
By H. BOVENSMANN, H. KNÖCKEL and E. TIEMANN 813

The magnetic structure of sodium biphenyl bistriglyme
By M. C. M. GRIBNAU and E. DE BOER 819

Vibration–translation energy transfer in a collision between an atom and a Morse oscillator
By J. RÉCAMIER A. and M. BERRONDO 831

Effect of electric field on internal vibration frequencies. Infrared analysis of CO_2 adsorbed in A zeolites
By A. M. GOULAY, F. CLAIRET and E. COHEN DE LARA 845

Structural studies of cyclohexane, C_6D_{12}, by neutron diffraction. II. The plastic crystal phase
By H. FARMAN, L. O'MARD, J. C. DORE and M.-C. BELLISSENT-FUNEL 855

Path integral simulation of the free energy of (Lennard-Jones) neon
By J. J. MORALES and K. SINGER 873

Theory and computer simulations of heteronuclear diatomic hard-sphere molecules (hard dumbbells)
By A. L. ARCHER and G. JACKSON 881

Molecular dynamics investigation of the inter- and intramolecular motions in liquid methanol and methanol–water mixtures
By G. PÁLINKÁS, I. BAKÓ, K. HEINZINGER and P. BOBB 897

Geometrical analysis of the structure of simple liquids: percolation approach
By Y. I. NABERUKHIN, V. P. VOLOSHIN and N. N. MEDVEDEV 917

Research Notes

The solvation pressure in a system of fixed density
By C. XIAO and J. S. ROWLINSON 937

Effects of BSSE and d-orbital space in the calculation of the equilibrium geometry of CaF_2
By T. G. WRIGHT, E. P. F. LEE and J. M. DYKE 941

Aspects of J pathways in $|A]_n(\mathscr{S}_n)|AX]$ spin systems over partitional, or coherent superpositional, Liouville space bases involving intracluster coupling, or associated with coherence transfer in $|A \ldots X]$ ($I_i = \frac{1}{2}$) systems: further group theoretical considerations
By F. P. TEMME and J. P. COLPA 953

NUMBER 5—10 AUGUST 1991

Giant gold clusters stabilized by triphenylphosphine ligands. Characterization by surface enhanced Raman and reflectance spectroscopy
By F. ZIMMERMANN and A. WOKAUN 959

The structure of fluids confined to spherical pores: theory and simulation
By M. CELLEJA, A. N. NORTH, J. G. POWLES and G. RICKAYZEN 973

Far-infrared optical constants of liquid acetonitrile at 238 to 343 K as measured with a synchrotron radiation source
By T. OHBA and S. IKAWA 985

Molecular dynamics study of local structure and reorientational dynamics in liquid acetonitrile
By T. OHBA and S. IKAWA 999

The influence of long range electrostatic forces on static properties of a quasi-Stockmayer fluid
By A. W. HERTZNER, M. SCHOEN and H. MORGNER 1011

Direct observation of the transitions $^2\Delta_{5/2}, v = 0 \rightarrow {}^2\Pi_{3/2}, v = 0$ and $^2\Delta_{5/2}, v = 0 \rightarrow {}^2\Delta_{3/2}, v = 1$ of the NiH radical by Faraday LMR, employing a CO overtone laser
By E. Bachem and W. Urban 1031

Vibration–rotation spectroscopy of the CrH radical in its $X^6\Sigma^+$ ground state by CO–Faraday laser magnetic resonance
By K. Lipus, E. Bachem and W. Urban 1041

Infrared diode laser spectroscopy of the electronic ground state of SnD
By U. Simon, M. Petri, W. Zimmermann, G. Huhn and W. Urban 1051

Incoherent neutron scattering study of the pseudorotational and diffusive motions of cyclopentane in condensed state
By M. Besnard, M. Fouassier, J. C. Lassegues, A. J. Dianoux and W. Petry 1059

Chemical shielding anisotropy of ^{13}C in $CH_3{}^*CN$ determined by NMR spectroscopy of the dielectrically oriented molecule
By L. Huis, F. J. J. de Kanter and C. Maclean 1077

***Ab initio* study of NO_2 Part III. Potential energy functions for the two lowest $^2A'$ states in both the diabatic and adiabatic representations**
By G. Hirsch, R. J. Buenker and C. Petrongolo 1085

Fermi resonance in liquid methyl bromide
By A. Bródka and R. Wrzalik 1101

Monte Carlo calculations of adsorbate placement and thermodynamics in a micropore: Xe in NaA
By P. R. Van Tassel, H. T. Davis and A. V. McCormick 1107

Molecular dynamics algorithm for flexible molecules using normal coordinates
By M. Buchner and B. M. Ladanyi 1127

On the effects of association in the statistical theory of ionic systems. Analytic solution of the py–msa version of the Wertheim theory
By M. F. Holovko and Yu. V. Kalyuzhnyi 1145

Convergence and efficiency of the valence bond self-consistent field method
By J. H. Van Lenthe, J. Verbeek and P. Pulay 1159

Research Notes

Simplified calculation of quantum corrections to the virial coefficients of hard convex bodies
By E. A. Mason, J. J. Siregar and Ying Huang 1171

Density functional theories for classical homogeneous systems
By Soon-Chul Kim 1179

NUMBER 6—20 AUGUST 1991

Vibration–rotation coordinates and kinetic energy operators for polyatomic molecules
By M. J. Bramley, W. H. Green, Jr. and N. C. Handy 1183

A study of the ground electronic state of disulphane
By Ming-der Su, A. Willetts, M. J. Bramley and N. C. Handy 1209

***Ab initio* static polarizabilities and multipole moments of I_2**
By G. Maroulis and A. J. Thakkar 1235

Molecular axis orientation and transitional path effects in the rotational structure of multiphoton transitions
By C. Maïnos 1241

Theory of rotational line strengths in coherent anti-Stokes Raman spectroscopy
By B. Attal-Trétout, P. Monot and K. Müller-dethlefs 1257

Surface segregation of a binary liquid mixture as studied by metastable impact electron spectroscopy
By H. Morgner, J. Oberbrodhage, K. Richter and K. Roth 1295

On the solvent frequency shift
By J. G. Powles, S. Murad, D. P. Sethi and P. V. Ravi 1307

Molecular dynamics simulation of solid biphenyl
By A. Baranyai and T. R. Welberry 1317

A molecular dynamics study of electric field gradients in condensed B-DNA systems
By T. R. Forester 1335

On the computer simulation of highly polar fluids using large systems
By P. G. Kusalik 1349

An ESR study of ion pairing in solutions of the alkali metal salts of tetracyanoquinodimethan (TCNQ) and tetrafluorotetracyanoquinodimethan ($TCNQF_4$)
By T. Maruo, R. D. Rataiczak and M. T. Jones 1365

Angular distributions of reactive scattering arising from persistent complexes with asymmetric top transition states
By D. J. Smith and R. Grice 1371

Molecular dynamics simulations of wetting and drying in LJ models of solid–fluid interfaces in the presence of liquid–vapour coexistence
By P. Adams and J. R. Henderson 1383

The onset of disorder on a surface with a step
By H. Xu and R. M. Lynden-Bell 1401